Topological Mott insulators of ultracold atomic mixtures induced by interactions in one-dimensional optical superlattices

Zhihao Xu[1] and Shu Chen[1,*]

[1]*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

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We present exactly solvable examples that topological Mott insulators can emerge from topologically trivial states due to strong interactions between atoms for atomic mixtures trapped in one-dimensional optical superlattice systems. The topological Mott insulating state is characterized by nonzero Chern number and appears in the strongly interacting limit as long as the total band filling factor is an integer, which is not sensitive to the filling of each component. The topological nature of the Mott phase can be revealed by observing the density profile of the trapped system. Our results can be also generalized to the multi-component atomic systems.

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Introduction.- Topological band insulators have attracted great attention in condensed matter physics since they were discovered in spin-orbit coupled two-and three-dimensional systems [1, 2]. As the topological insulator (TI) is expected to be robust against weak perturbations, it is important to consider the effect of interactions on the topological band insulators [3–6]. Although generally a strong interaction may open the energy gap and break the TI, there exists a class of topological insulator called as the topological Mott insulator, where the interaction effects are responsible for TI behavior [7]. The topological Mott phases have attracted increasing attention [8–10] since the concept is proposed as interaction plays a crucial role in the formation of both the Mott phase and nontrivial topology. As almost all these results based on the mean-field approximation, examples with the interaction effect counted exactly is particularly important for our understanding of the topological Mott insulator.

In this work, we explore the realization of topological Mott phases in cold atomic systems trapped in one-dimensional (1D) quasi-periodic optical lattices, which can be generated by superimposing two 1D optical lattices with commensurate or incommensurate wavelengths [11–13]. Cold atomic systems in 1D quasi-periodic lattices have been extensively studied [14–17] with a focus on the Anderson localization [12]. However, their nontrivial topological features are recognized only very recently [18, 19]. Particularly, with the experimental observation of the topological edge states in 1D photonic quasi-crystals [19] there is a growing interest in the study of topological properties in the 1D quasi-periodic lattices [20–25]. It has been shown that the free fermion system with its sub-bands being fully filled is a topological nontrivial insulator, which can be characterized by a nonzero Chern number in the extended two-dimensional (2D) parameter space [18]. In this work, we study the interacting multi-component atomic mixtures in the 1D superlattice with its sub-bands are partially filled by atoms. In the absence inter-component interaction, the system may be a Fermi metal, a Bose superfluid or their mixture, depending on the component of mixture being fermion or boson. We find that a topological Mott insulator may emerge in the strongly interacting regime if the total band filling is an integer. This conclusion is exact in the infinitely strong interaction limit as it is based on an exact mapping which relates the many-body wavefunction of two-component mixture to the wavefunction of free fermion system. Our study provides a simple way to realize the topological Mott insulator in cold atomic systems and may deepen our understanding of the topological Mott insulator.

Interacting atomic mixtures in optical superlattices.- We consider the 1D atomic mixtures loaded in a bichromatic optical lattice [11–13], which is described by $H = H_0 + H_I$ with

$$H_0 = -t \sum_{i,\sigma=\uparrow,\downarrow} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} + \text{H.c.}) + \sum_{i,\sigma=\uparrow,\downarrow} V_i \hat{n}_{i,\sigma} \quad (1)$$

and

$$H_I = U \sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \sum_i \frac{1}{2} U_\sigma \hat{n}_{i,\sigma} \left(\hat{n}_{i,\sigma} - 1\right), \quad (2)$$

where $V_i = \lambda\cos(2\pi\alpha i + \delta)$ with λ controlling the strength of commensurate potential, α tuning the modulation period and δ being an arbitrary phase, $c_{i,\sigma}$ are bosonic or fermionic annihilation operators localized on site i, and $n_{i\sigma} = c^{\dagger}_{i_\sigma} c_{i_\sigma}$. Here $\sigma = \uparrow, \downarrow$ denotes the pseudo-spin index of two components of atomic mixtures, which can be either fermion or boson. The interaction parameter U denotes the inter-component interaction strength and U_σ denotes the intra-component interaction strength between bosonic atoms. For the Fermi-Fermi mixture, $U_\sigma = 0$ due to the Pauli exclusion. For the Fermi-Bose mixture, one of U_σ is zero if σ denotes the fermion component. In principle, both U and U_σ can be tuned experimentally by the Feshbach resonance. The hopping amplitude t is set to be the unit of the energy ($t = 1$).

In the absence of interaction, i.e., $H_I = 0$, the eigenvalue equation, namely the Harper equation, is given by

$$-[\phi_n(i+1)+\phi_n(i-1)]+\lambda\cos(2\pi\alpha i+\delta)\phi_n(i) = \epsilon_n\phi_n(i), \quad (3)$$

where $\phi_n(i)$ denotes the single particle wave function and ϵ_n the n-th single particle eigenenergy. For a superlattice with $\alpha = p/q$ (p and q are co-prime integers), the system has a unit cell of q sites and the single-particle spectrum is split into q bands, which also changes periodically as the phase δ varies from 0 to 2π. Given that the number of σ-component atoms is N_σ and the number of lattice sites is L, we define the component-depending band filling factor ν_σ as $\nu_\sigma = N_\sigma/N_{cell}$ with $N_{cell} = L/q$ being the number of primitive cells. For a Fermi system, the system with the band filling factor $\nu_\sigma = m$ (m is an integer smaller than q) corresponds to a band insulator with the lowest m bands being fully filled by the σ-component fermion. Such a band insulator has been demonstrated to be characterized by a nontrivial topological Chern number in a 2D parameter space spanned by momentum and the phase of δ [18].

In the following calculation we shall consider the two-component system with fractional filling factors $\nu_\uparrow$ and $\nu_\downarrow$ but the total band filling factor $\nu = \nu_\uparrow + \nu_\downarrow$ being an integer. For a free two-component Fermi system with such a filling, the sub-band is only partially filled and the system is a topologically trivial conductor. We shall show that a Mott phase can emerge from the conducting phase with an integer total filling factor when the interaction effect is considered.

Emergence of Mott phase for the Fermi-Fermi mixture.- To give a concrete example, we first consider the Fermi Hubbard model in the superlattice, i.e., the Hamiltonian (1) and (2) with $U_\sigma = 0$. We consider the case with $\alpha = 1/3$ and $\nu = 1$, for which $n = N/L = 1/3$. We calculate the charge gap, which is defined as $\Delta = [E_0(N+1)+E_0(N-1)]/2 - E_0(N)$, by numerically diagonalizing the Hamiltonian, where $E_0(N)$ represent the ground state for the N-atom system. In the Fig.1a, we show the charge gap versus the repulsive interaction strength U for the equal-mixing case with $\nu_\uparrow = \nu_\downarrow = 1/2$. It is shown that the charge gap increases with increasing U and tends to a constant in the large U limit. For systems with different sizes, we find the charge gap in the large U limit approaches to the half size of the band gap Δ_b between the lowest band and the second one. The numerical results suggest that a Mott insulator is emergent in the strongly interacting limit as the gap is induced by the repulsive interaction between fermions of different components.

Next we calculate the charge gap versus the repulsive interaction strength U for various U' for the equal-mixing Fermi-Bose mixture. Here we use U' to represent intra-component boson-boson interaction strength for the two-component Fermi-Bose mixture. As shown

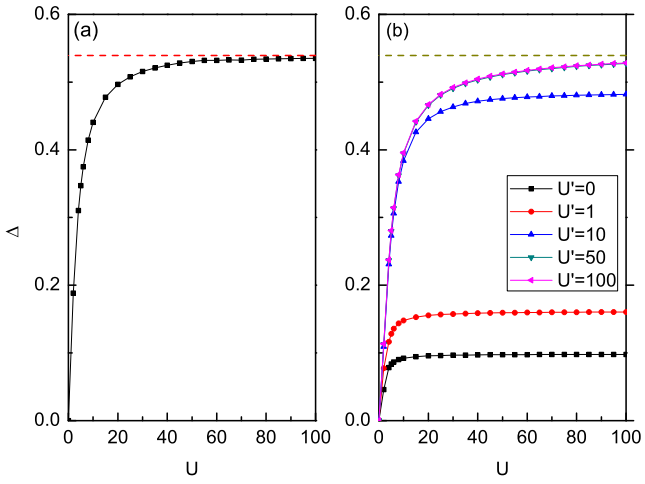

FIG. 1: (Color online) The charge gap versus the interaction strength U for equal-mixing Fermi-Fermi system (a) and Fermi-Bose system (b) with $\alpha = 1/3$, $\lambda = 1.5$, $\delta = 0$, $N_\uparrow = N_\downarrow = 2$ and $L = 12$ under periodic boundary conditions (PBC).

in Fig.1b, with the increase in the boson-boson interaction strength, the charge gap increases and the curve approaches the curve of Fermi-Fermi mixture. In the limit of hard-core boson, i.e., $U_\sigma \to \infty$ for the Bose-Bose mixture and $U' \to \infty$ for the Fermi-Bose mixture, both the Bose-Bose Hubbard model and Bose-Fermi Hubbard model can be mapped into the Fermi Hubbard model by extended Jordan-Wigner transformations [26]. Therefore, the above discussion on the Fermi-Fermi mixture can be directly applied to hard-core-boson limit of the Bose-Bose and Fermi-Bose mixtures. For these systems with $\nu = 1$, the Mott phase is emergent with increasing the strength of inter-specie repulsion U.

Atomic mixtures in the strongly interacting limit.- The emergence of the charge gap for the superlattice system with integer band filling factor can be clearly understood in the strongly interacting limit. In the infinitely strong repulsion limit, $U \to \infty$, we can construct the many-body wavefunction of the interacting fermion system exactly by using the hard-core contact boundary condition [27] and group theoretical methods [28]. Combining with the Pauli exclusion principle, the effect of an infinitely strong interaction can be reduced to a hard-core contact boundary condition $\Psi(x_1,\sigma_1;\cdots;x_N,\sigma_N)\ |_{x_i=x_j} = 0$, which does not depend on spin configurations. According to Ref. [28], the many-body wave function of the system can be represented as $\Psi = \Psi_A\Psi_S$, where the spatial wave function Ψ_A is composed of Slater determinant of $N = N_\uparrow + N_\downarrow$ orbitals $\phi_1(x),\cdots,\phi_N(x)$, given by

$$\psi_A(x_1,\ldots,x_N) = (N!)^{-\frac{1}{2}} det[\phi_n(x_i)]_{i=1,\ldots,N}^{n=1,\ldots,N} \quad (4)$$

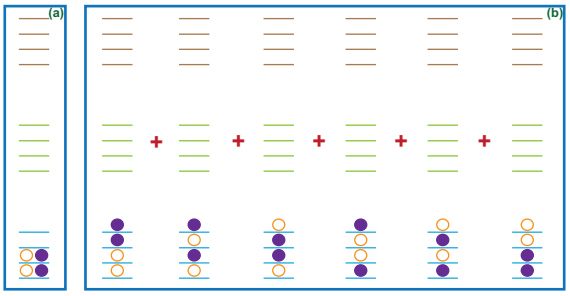

FIG. 2: (Color online) Schematic diagram for the ground state energy level occupations for system with $\alpha = 1/3$, $N_\uparrow = N_\downarrow = 2$ and $L = 12$. (a) is for $U = 0$ and (b)is for $U \to \infty$.

with $\phi_n(x)$ ($x = ia$ with a the lattice constant) the eigenstate of the single particle Hamiltonian H_0, whereas Ψ_S is a mapping function composed of linear combination of production of sign function and basis tensor of spin, whose explicit form is given in Ref. [28]. Effectively, the effect of infinite repulsion is to generate a Pauli exclusion between different components of fermions. Such an effect has been recently observed by the experiment in a two-particle system with tunable interaction using two fermionic ^{6}Li atoms [29]. The ground state of the system in the limit of $U \to \infty$ is composed of states with the lowest N single particle states occupied, and the ground energy is given by $E_0 = \sum_{n=1}^{N} \epsilon_n$. As a comparison, the ground energy of the free fermion system is given by $E_0 = \sum_{n=1}^{N_\uparrow} \epsilon_n + \sum_{n=1}^{N_\downarrow} \epsilon_n$.

Now we can understand the formation of Mott phase in optical superlattices by considering the limit case with infinitely strong interaction. As illustrated in Fig.2, for the superlattice with $\alpha = 1/3$, the energy levels split into three bands. When $U = 0$, the lowest band is only partially filled for $\nu_\uparrow = \nu_\downarrow = 1/2$. However the lowest band is fully filled in the limit of $U \to \infty$ corresponding to $\nu = 1$ as each energy level can only be occupied by a fermion with either spin up or spin down, and consequently a charge gap is opened. According to the definition of charge gap, the charge gap equals to half of the band gap as adding a fermion costs the energy of Δ_b. This is consistent with the numerical result displayed in Fig.1. For a general case with $\alpha = 1/q$, the energy levels are composed of q bands. As long as $\nu = m$ with $m = 1, \cdots, q-1$, a Mott insulator is formed as $U \to \infty$. For a fractional ν, for example, $\nu < 1$, the lowest band is not fully filled even in the strong interaction limit, and thus no finite charge gap is opened.

The above discussion can be directly applied to the Bose-Bose mixture and Fermi-Bose mixture with infinitely strong inter-component and intra-component interaction. As $U \to \infty$ and $U_\sigma \to \infty$, the effect of the infinitely strong interaction can be also reduced to the hard-core contact boundary condition $\Psi(x_i = x_j) = 0$, which enforces an effective Pauli exclusion to hard-core

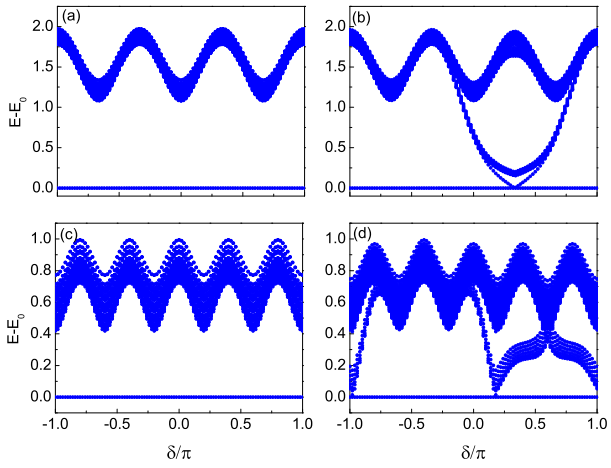

FIG. 3: (Color online) Low-energy spectrum versus δ for two-component mixture systems with $\lambda = 1.5$ and different α in the infinitely repulsive limit. (a) $\alpha = 1/5$, $N = 30$, $L = 90$ under PBC; (b) $\alpha = 1/3$, $N = 30$, $L = 91$ under OBC; (c) $\alpha = 1/5$, $N = 40$, $L = 100$ under PBC; (d) $\alpha = 1/5$, $N = 40$, $L = 101$ under OBC.

bosons and between different components of atoms. Consequently, the exact wave function of the system can be also represented as $\Psi = \Psi_A \Psi_S$, where Ψ_A is identical to the expression of (4), but Ψ_S has different form for different kind of mixtures [27, 28, 30]. For the Bose-Bose mixture, $\Psi_S = \prod_{1 \le i,j \le N} sgn(x_i - x_j)$, where $sgn(x)$ is the sign function. The explicit form of the mapping function Ψ_S for the Fermi-Bose mixture is given in Ref. [27].

Topological feature of the Mott phase.- To characterize the topological feature of the many-body states, it is convenient to introduce a generalized boundary phase θ by applying the twist boundary condition along the 1D chain. In the 2D parameter space of (θ, δ), we can calculate the Chern number of the many-body state, which is defined as an integral invariant $C = \frac{1}{2\pi} \int d\theta d\delta F(\theta, \delta)$, where $F(\theta, \delta) = \mathrm{Im}(\langle \frac{\partial \Psi}{\partial \delta} | \frac{\partial \Psi}{\partial \theta} \rangle - \langle \frac{\partial \Psi}{\partial \theta} | \frac{\partial \Psi}{\partial \delta} \rangle)$ is the Berry curvature [31, 32]. For the two-component mixtures in the strongly interacting limit, we notice that the many-body wave functions under the twist boundary condition can be represented as $\Psi(\theta, \delta) = \Psi_A(\theta, \delta)\Psi_S$, where only Ψ_A varies with the change of θ and δ, whereas Ψ_S is independent of θ and δ as it is composed of combination of production of sign functions. This greatly simplify the calculation of the Chern number as $F(\theta, \delta) = \mathrm{Im}(\langle \frac{\partial \Psi_A}{\partial \delta} | \frac{\partial \Psi_A}{\partial \theta} \rangle - \langle \frac{\partial \Psi_A}{\partial \theta} | \frac{\partial \Psi_A}{\partial \delta} \rangle)$, where Ψ_A is given by Eq.(4). Consequently, in the strong interacting limit, the Chern number for atomic mixtures composed of $N_\uparrow$ and $N_\downarrow$ two-component atoms is identical to the Chern number of the system composed of N free fermions. For the strongly interacting atomic mixtures on the superlattice

with $\alpha = 1/3$, the Mott insulators are formed when $\nu = 1$ and $\nu = 2$, corresponding to states with Chern number $C = 1$ and $C = -1$. These Mott insulators are thus topologically nontrivial insulators.

According to the bulk-edge correspondence in general topological insulators, one may expect that the topological Mott insulators should display nontrivial edge states for the system with open boundary conditions (OBC). To see it clearly, we display the excitation spectrum for mixture systems in the infinitely strong repulsion limit with $\nu = 1$, $\alpha = 1/3$ and $\nu = 2$, $\alpha = 1/5$ in Fig.3 versus the phase δ. The system with $\nu = 1$ and $\alpha = 1/3$ is a topological Mott insulator characterized by the Chern number $C = 1$, whereas the topological Mott insulator corresponding to $\nu = 2$ and $\alpha = 1/5$ is characterized by the Chern number $C = 2$. As shown in Fig. 3a and Fig. 3c, there is an obvious gap between the ground state and the first excited state for systems with PBC. However, as shown in Fig. 3b and Fig. 3d, edge states appear in the gap regimes for systems with OBC. As the phase varies from $-\pi$ to π, the edge states connect the ground state to the excited band. When the interaction deviates from the infinite limit, despite of the exact mapping no longer holding true, our numerical results indicate that the topological Mott phase still exits. As shown in Fig.4, the excitation spectrum for the system with $U = 100$ exhibits almost the same behavior as shown in Fig.3b. Even when the interaction strength decreases to $U = 5$, the spectrum still has similar structure. The main difference is that the ground state levels are broadened due to spin fluctuations and the degeneracy of ground states in the infinite interaction limit is lifted for finite interactions.

Our results can be directly extended to the general multi-component atomic systems trapped in 1D superlattices. When the inter-specie and inner-specie interactions between atoms go to the strongly interacting limit, an effective Pauli exclusion between atoms arises. Therefore, a topological Mott insulator is expected to appear in the topologically nontrivial superlattice as long as the total filling factor $\nu = \sum_\kappa \nu_\kappa$ is an integer, where κ is the component index of the multi-component atomic mixture.

Experimental detection.- A possible way to observe the topological Mott insulator is to detect the density distribution of the superlattice systems with an external confining potential, i.e., V_i in Eq.(1) is replaced by $V_i = \lambda\cos(2\pi\alpha i + \delta) + V_H(i - i_0)^2$, where V_H is the strength of the harmonic trap with i_0 being the position of trap center. In Fig.5, we show the local average density distribution of two-component fermions with imbalance populations trapped in the optical superlattice with a harmonic trap. The local average density is defines as $\rho_i = \sum_{j=-M}^{M} n_{i+j}/(2M+1)$ with $M \ll L$ [18], where $n_i = \langle\hat{n}_{i,\uparrow}\rangle + \langle\hat{n}_{i,\downarrow}\rangle$. In the strongly interacting limit, two plateaus with $\rho = 1/3$ and $\rho = 2/3$ appear for $\alpha = 1/3$, whereas four plateaus with $\rho = 1/5, 2/5, 3/5, 4/5$ appear for $\alpha = 1/5$. We note that locations of plateaus appear at $\rho(\alpha) = \alpha, 1-\alpha, 2\alpha, 1-2\alpha, 4\alpha, 1-4\alpha, ...$, if the values are in the range of $(0, 1)$. For contrast, the density profiles for $U = 0$ do not exhibit these plateaus. The Chern number can thus be deduced from the plateau distribution by using the Streda formula [18, 33] $C = \frac{\partial\rho(\alpha)}{\partial\alpha}$. It is straightforward to get $C = 1, -1$ for $\rho_i = \alpha, 1-\alpha$ and $C = 2, -2$ for $\rho_i = 2\alpha, 1-2\alpha$.

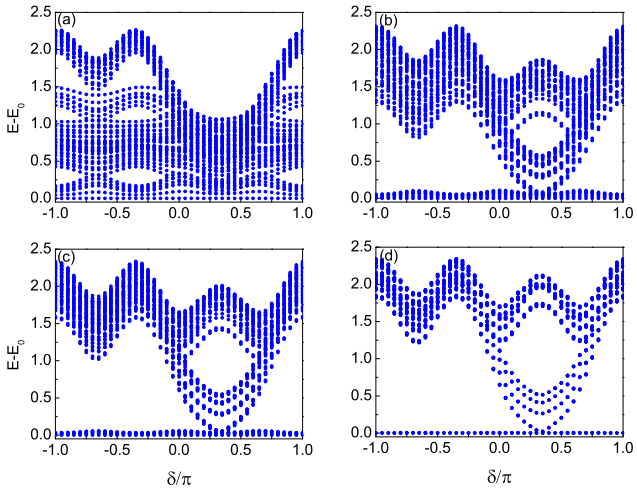

FIG. 4: (Color online) Low-energy spectrum versus δ for the Fermi-Fermi mixture with $\alpha = 1/3$, $\lambda = 1.5$ $N_\uparrow = N_\downarrow = 2$, $L = 13$ and various U under open boundary condition. (a) $U = 1$, (b) $U = 5$, (c) $U = 10$ and (d) $U = 100$.

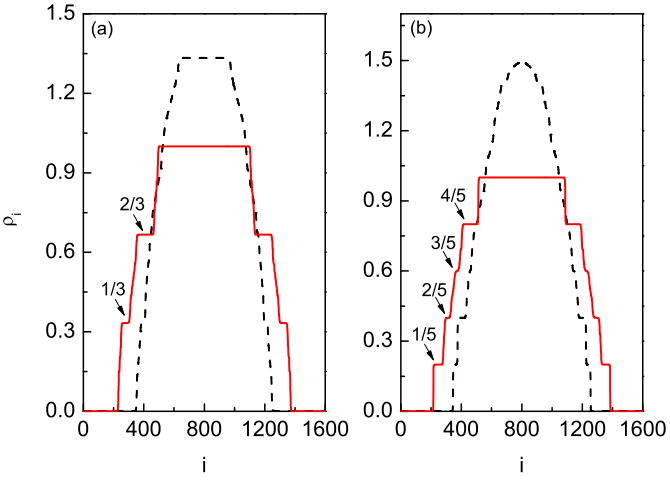

FIG. 5: (Color online) The local average density distributions for the superlattice with $\alpha = 1/3$ (a), and $\alpha = 1/5$ (b) trapped in the harmonic trap. The system is with 1600 sites, $N_\uparrow = 400$, $N_\downarrow = 500$, $\lambda = 1.5$, $\delta = 0$ and $V_H = 2 \times 10^{-6}$. The dot line is for the case of $U = 0$ and the solid line is for the case of $U \to \infty$. Here, we take $M = (q-1)/2$.

Summary.- In summary, we studied the realization of topological Mott insulators in interacting atomic mixtures trapped in 1D optical superlattices. We give a clear interpretation for the formation of topological Mott insulator by using an exact mapping, which relates the many-body wavefunction of atomic mixtures in the strongly interacting limit to that of the free fermion system. The topological Mott insulator displays nontrivial edge states and can be characterized by a nonzero Chern number. The topological feature of the Mott insulator can be revealed by detecting plateaus of density profiles of the trapped lattice systems. Our results pave the way for experimentally studying topological Mott insulators in 1D optical lattices.

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* Electronic address: schen@aphy.iphy.ac.cn

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